

XAFS determination of local environment about Sr in CMR material, $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$

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Introduction

Sr doped lanthanum manganites $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ show colossal magnetoresistance effects that strongly depends on x [1]. A number of recent studies show the existence of charge, orbital, and spin ordering, and a number of anomalies have been observed in transport or magnetic properties. These properties have been generally been explained assuming that the sample composition is homogeneous through the entire sample. However, since these materials are synthesized from two different source materials, there arises a question about the homogeneity of the composition at the atomic scale around the La and Sr sites. Here we report XAFS studies of Sr K-edge to determine the local coordination of La around Sr atoms as a function of alloy composition.

Methods and materials

The sintered compounds of LaSrMnO_3 ($x=0.075$, 0.225 , and 0.325) were ground to powders and sieved to 400 mesh ($< 30\mu\text{m}$ particle size). These powders are brushed to scotch tapes and several folds of them were used as a sample. They were mounted in a DISPLEX closed cycle helium cryostat and measured at 10K. All the measurements were performed at MRCAT (ID-10) at Advanced Photon Source(APS) in a transmission geometry. The synchrotron beam from undulator was monochromatized by a double Si crystal monochromator. A harmonic rejection mirror was used to eliminate the higher energy x-rays. The beam was defined by a pair of motorized slits and incident to the sample. Both incident and transmitted beam were detected by gas filled ion chambers. All the measurement system including the cryostat were equipped at the beamline. Each sample was usually measured three times to ensure the repeatability of the measurements and they are averaged out to have better signal to noise ratio especially at higher electron momentum transfer (k (\AA^{-1}) region.

Results

Figure 1 shows the Sr K edge XAFS of the $x=0.225$ sample as an example of the data quality. Three scans are averaged.

Figure 2 shows $k^3\chi$ Fourier transform of $x=0.225$ data together with the FEFF calculation of the same structure with different ratio of Sr/La coordination at the first (Sr/La)=1/5, 2/4, and 3/3 shell. Here the total coordination at this site is 6. We note that the intensity at

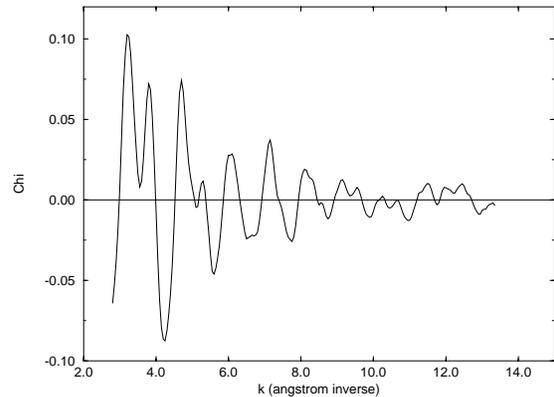


Figure 1: $\chi(k)$ of $x=0.225$ at 10K. Three scans are averaged.

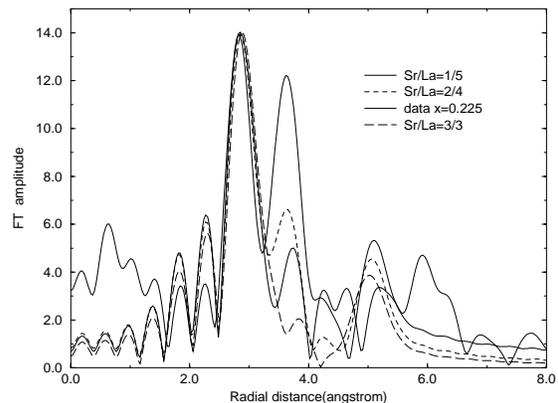


Figure 2: Fourier transform of $k^3\chi$ for $x=0.225$ (thick solid line), and FEFF calculation with the ratio of (Sr/La)=1/5(thin solid), 2/4(short dashed), and 3/3 (long dashed) at the first La/Sr shell. In the calculation, the intensity at $R=3.6\text{\AA}$, is strongly dependent on this ratio because of the difference of the backscattering amplitude of La and Sr. The data locates between Sr/La=2/4 and 3/3, although between 1/5 and 2/4 is expected from the composition of the sample.

$R=3.6\text{\AA}$, the distance between Sr and La/Sr site, should be strongly dependent on the ratio of La/Sr coordination numbers since La is much stronger backscatter than Sr. That is, if the Sr is preferentially coordinating around the Sr, the intensity should appear smaller. We see from this figure that the data is between Sr/La=2/4 and 3/3 although from the composition, between Sr/La=1/5 and 2/4 would be expected if the sample is homogeneous. The appropriate estimation of the factors affecting the intensity of the Fourier transform such as Debye Waller factor and S_0^2 should be necessary for the precise determination of the coordination numbers, however, we would naively say that the Sr is preferentially located at the first La/Sr site.

Discussion

We performed XAFS for $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ with three different Sr content. It turned out that the XAFS is suitable tool to determine the coordination of La/Sr around Sr atom. Further improvement of the data quality, especially higher S/N ratio to higher k (up to 16\AA^{-1}) and systematic studies about x covering from very low Sr concentration such as $x=0.02$ to high concentration such as $x=0.5$ should be necessary for the discussion of the coordination number around Sr environment. Also, the quantitative analysis should be performed by the comparison with the simulations from the FEFF 6.01 program [2] and by profile fitting by FEFFIT program [3].

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